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A Generalized ICE Method for Chemically Reactive Flows in Combustion Systems*

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A generalization of the Implicit Continuous-Fluid Eulerian (ICE) technique has been developed for the calculation of fluid flows in the presence of rapid exothermic chemical reactions typical of combustion environments. Systematic errors occur in the conventional operator splitting solution technique for the case of exothermic chemically reactive flows. These errors are the result of a biasing in the order in which the ICE and its derivative techniques solve the relevant conservation equations. Exothermic chemical reactions and thermal energy transport play important roles in determining the time-advanced pressure in the implicit treatment of the hydrodynamics for combustion environments, and the ICE models do not properly include these effects. The generalized ICE method presented corrects these systematic errors by properly coupling all of the operators which can have significant effects on the fluid pressure. The conventional solution method and the generalized method are each applied to a sample problem in order to illustrate the differences in the models.

INTRODUCTION

There has been a great deal of progress in recent years in the development of implicit methods for the solution of problems in fluid dynamics. Much of this work has been reviewed by Harlow [1]. Many of the implicit methods in use have been based to some degree on what was named the ICE (Implicit Continuous-Fluid Eulerian) method of Harlow and Amsden [2]. In the original ICE method, the continuity and momentum equations are coupled together and solved simultaneously, using the equation of state to relate the time-advanced pressure to the time-advanced fluid density. After those equations are solved, the energy conservation equation is solved explicitly in time, decoupled from the continuity and momentum equations.

The ICE method has proved to be an exceedingly versatile and useful basis upon which to build numerical models for a variety of physical applications. The RICE program [3] added operators, also decoupled from the continuity and momentum equations, to account for chemical kinetics rate equations and transport of chemical species. Another very important related development was the addition of the Arbitrary-Lagrangian-Eulerian (ALE) technique of Hirt *et al.* [4, 5] to permit use of the ICE

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method in extremely general finite difference meshes. The combined ICED–ALE programs still use the same operator splitting method of the ICE technique for the continuity and momentum equations. Pracht [6] has extended the ICED–ALE model to three dimensions. Harlow and Amsden [7] incorporated a multifluid model into the ICED–ALE framework for multiphase calculations. Gal-Chen and Somerville [8] included surface topography for atmospheric flows. Sanford and Anderson [9], and Sanford *et al.* [10] have coupled an implicit Monte Carlo radiation transport model to the ICE and ICED–ALE models. Brackbill and Pracht [11] used ICED–ALE as the basis for MHD calculations, including both the fluid and magnetic pressure in the fluid flow calculations. In recent applications there appears to be some concern that the energy equation can have an important impact on pressure variations over the hydrodynamic time step. In modeling low Mach-number, homogeneous two-phase flows, Ramshaw and Trapp [12] coupled the energy equation to the continuity and momentum equations, but the energy equation was solved explicitly in time and there was no iteration to correct the effects of energy transport on the time-advanced pressure.

In all of the above models, the basic solution strategy is patterned after that of the ICE method, in which the time-advanced pressure and density are related through an equation of state. The energy equation is not solved simultaneously and implicitly with the continuity and momentum equations. These treatments therefore assume that changes in the fluid pressure in each computational cell are due primarily to density changes and that pressure changes due to changes in internal energy, temperature, or other physical processes are relatively small. This situation prevails in a large number of applications for which the ICE method was designed or modified, including problems in which energy diffusion rates and energy deposition rates are small. If the change in internal energy is small, then the final correction to the pressure from the solution of the energy equation is also small; the pressure which was used in the solution of the hydrodynamics equations was in fact a good estimate of the true time-advanced pressure.

However, this assumption in the ICE method is not always valid. Situations arise where the internal energy density can change as a result of rapid energy deposition in the fluid. In some cases the ICE method can be adjusted appropriately to deal with this problem. As noted, Ramshaw and Trapp [12] used the energy equation, solved explicitly in time, to estimate the change in pressure over the time step due to energy exchanges in two-phase flows. O'Rourke and Bracco [13] have used the rate of chemical reaction energy deposition, again evaluated explicitly in time, to help estimate the pressure changes in applications of the RICE program to combustion problems.

In most combustion problems the calculation of the fluid dynamics properties of the reacting fluid is complicated by the fact that rapid exothermic chemical reactions are taking place in portions of the combustion chamber. Since the mass and momentum flux terms in an implicit formulation depend on having an accurate estimate of the time-advanced pressure, it is essential to include in the implicit, coupled fluid dynamics equations all of the effects and operators which could significantly affect that pressure. The ICE family of programs is being used increasingly in combustion modeling programs [13–17] and it is important to examine the suitability of the method to these applications. We find that use of the ICE technique can result in systematic errors in many combustion calculations. The ICE method, however, is very attractive as a general outline. The purpose of this paper is to describe a generalization of the ICE method which avoids these systematic errors and to demonstrate its use in a typical combustion application. Finally, some guidelines are presented, indicating in what circumstances the ICE method may be used without modification, in any class of applications.

MODEL DEVELOPMENT

The equations for conservation of mass, momentum, and energy are exactly the same as in the original ICE formulation [2]. In order to keep the description simple we illustrate this discussion with the one-dimensional equations. The generalization to two and three dimensions will be obvious. These equations are

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = \tau \frac{\partial^2 \rho}{\partial x^2}, \tag{1}$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} = -\frac{\partial (P+Q)}{\partial x}, \tag{2}$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho u E}{\partial x} = \frac{\partial}{\partial x}\left[B\mu \frac{\partial I}{\partial x} - (P+Q)\,u\right], \tag{3}$$

where

$$Q \equiv -\lambda \frac{\partial u}{\partial x} \tag{4}$$

and

$$E \equiv I + u^2/2. \tag{5}$$

The above terms are discussed in Ref. [2], and the spatial and time centering conventions from [2] also apply. In the ICE and related methods, the continuity and momentum equations, the difference equation analogs of Eqs. (1) and (2), are solved simultaneously. The equation of state is used to relate the time-advanced pressure $\bar{P}$ and the time-advanced density ρ^{n+1},

$$\bar{P} = P^n + c^n(\rho^{n+1} - \rho^n), \tag{6}$$

where

$$c^n = (\partial P/\partial \rho)^n, \tag{7}$$

to arrive at the equation to be solved for $\bar{P}$. In one dimension, this equation is

$$\bar{P}_i/c_i^n = [\theta\phi(\Delta t)^2/(\Delta x)^2](\bar{P}_{i-1} + \bar{P}_{i+1} - 2\bar{P}_i) + G_i, \tag{8}$$

in which G_i involves only terms available at the beginning of the time step. The commonly used expression for pressure in most combustion applications is the multispecies ideal gas equation of state

$$P = \rho RT \sum_{l=1}^{L} \frac{Y_l}{A_l}, \tag{9}$$

in which R is the gas constant, A_l is the molecular weight of chemical species l, Y_l is the mass fraction (ρ_l/ρ) of species l, and T is the temperature. If we expand the pressure about the values at the previous time t^n, we have

$$\begin{aligned} &= P^n + \left(\frac{\partial P}{\partial \rho}\right)^n (\rho^{n+1} - \rho^n) + \left(\frac{\partial P}{\partial T}\right)^n (T^{n+1} - T^n) \\ &\quad + \sum_{l=1}^{L} \left(\frac{\partial P}{\partial Y_l}\right)^n (Y_l^{n+1} - Y_l^n). \end{aligned} \tag{10}$$

Note that the expression used in the ICE method, Eq. (6), includes only the first two terms on the right-hand side of Eq. (10). In the ICE program the pressure changes due to changes in temperature (or internal energy) are not included in the solution of Eq. (8). Since they are assumed to be small changes, the pressure variations due to internal energy are accounted for subsequent to the explicit solution of the energy equation. In the RICE code [3], in which chemical species transport equations and chemical kinetics equations are included, the last term on the right-hand side of Eq. (10) is also assumed to be small, and changes in pressure due to changes in composition are added explicitly after all other corrections to the pressure have been made.

The principle behind the ICE method is that the best possible estimate for the time-advanced pressure must be used in the momentum equation, Eq. (2). Therefore, all of the physical processes which can significantly affect that pressure must be coupled to the solution of the continuity and momentum equations. In combustion problems this requires that the energy equation and the species kinetics and transport equations be solved together with the continuity and momentum equations, rather than be solved subsequently as is done in the RICE code.

We begin the present formulation by estimating the time-advanced pressure, including the effects of the energy and chemical species conservation equations. The overall system of equations is nonlinear, and we will adopt an iterative solution method. We define an iteration index m such that ρ^m is the mth iterative approximation to ρ^{n+1}, and similarly for all other variables. For the first approximation when $m = 1$ we use values at the previous time step t^n. The time-advanced pressure is then expanded about the previous iterate, giving

$$\begin{aligned} \bar{P} &= P^m + \left(\frac{\partial P}{\partial \rho}\right)^m (\rho^{m+1} - \rho^m) + \left(\frac{\partial P}{\partial T}\right)^m (T^{m+1} - T^m) \\ &\quad + \sum_{l=1}^{L} \left(\frac{\partial P}{\partial Y_l}\right)^m (Y_l^{m+1} - Y_l^m). \end{aligned} \tag{11}$$

For $m = 1$ this is identical to Eq. (10). A higher-order Taylor series expansion for $\bar{P}$ might be used instead of Eq. (11) in order to account for the possibility of very strong coupling between changes in temperature and species concentrations and to improve the convergence of the iteration scheme. In practice the linearized Taylor series expansion is adequate for the applications which were studied. If the iteration scheme does not converge, the time step is reduced and that cycle is recomputed, but this procedure was rarely necessary for the combustion applications discussed below. Using values for all of the variables at the mth iterate, the energy equation and the chemical species equations, including kinetics, are solved for T^{m+1} and Y_l^{m+1}. We then define H_i^m as

$$H_i^m = G_i + \left(\frac{\partial P}{\partial T}\right)^m \frac{(T^{m+1} - T^m)}{c_i^m} + \frac{1}{c_i^m} \sum_{l=1}^{L} \left(\frac{\partial P}{\partial Y_l}\right)^m (Y_l^{m+1} - Y_l^m). \tag{12}$$

The equation to solve for $\bar{P}$ has now become

$$\bar{P}_i/c_i^m = [\theta\phi(\Delta t)^2/(\Delta x)^2](\bar{P}_{i-1} + \bar{P}_{i+1} - 2\bar{P}_i) + H_i^m. \tag{13}$$

Formally this equation is identical to Eq. (8), which is solved by the ICE family of programs except that the constant vector G_i has been replaced by H_i^m, which is held constant while Eq. (13) is solved. The same similarity holds for the two-dimensional case, so that the methods used by any ICE-related program could still be used, with the substitution of H_i^m for G_i. In the generalized method, just as in the ICE model, once $\bar{P}$ is known, ρ^{m+1} and $(\rho u)^{m+1}$ may be calculated immediately. An important improvement in the new formulation, however, is the fact that these new values for ρ^{m+1} and $(\rho u)^{m+1}$ include the simultaneous effects of all of the physical processes which can affect the pressure and the fluid flow properties. Finally, the pressure P^{m+1} is

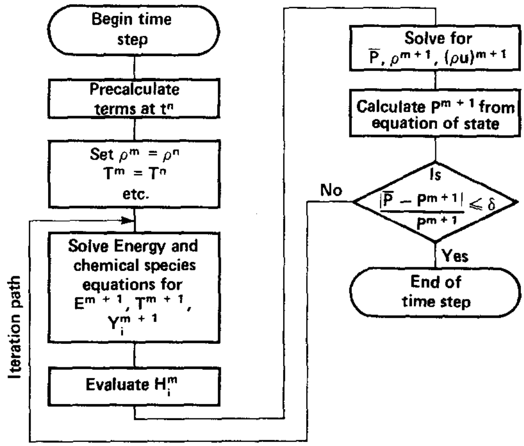

FIG. 1. Logical flowchart for solution of conservation equations using the generalized ICE model, showing the convergence test and iteration path.

computed and compared with P^m, the approximation at the previous iterate. Convergence is achieved when the corrections between one iteration and the next fall below some specified level. If convergence has not been reached, the latest iterative solutions are used to again solve the energy and chemical species equations and another iteration is computed. The overall structure of the iteration cycle is presented schematically in Fig. 1. The difference between this approach and that of ICE/RICE lies in the fact that we have included the effects of the energy equation and the chemical species equations inside the iteration loop, rather than solving them after the hydrodynamic equations have been solved.

EXAMPLE

To illustrate the properties of the generalized ICE method, a rather simple combustion problem was calculated using two different models. In one calculation the conventional operator splitting technique in the RICE program [3] was used, and in the other calculation the present generalized, coupled model was used. Both problems used identical initial conditions, chemical kinetic data, and transport coefficients. In this one-dimensional example, a combustion chamber having a linear dimension of 10 cm is filled initially with a stoichiometric mixture of fuel and oxidizer, which is assumed to have been compressed adiabatically to a density 10 times atmospheric density, so that the initial temperature of the gas is > 750 K and the pressure is 25 atm. The combustion is represented by a single-step exothermic chemical reaction. Initially the temperature, density, composition, and pressure are all spatially uniform. The mixture is ignited at one side of the chamber, and a turbulent planar deflagration wave moves across the chamber, consuming the reactant species and releasing energy. The turbulent Lewis number of each of the chemical species is set equal to unity, so that energy and species diffusion are assumed to be controlled by the diffusion of turbulent eddies. In these examples the turbulent diffusivity μ/ρ was set equal to a constant value of 500 cm^2/sec. Typical zone widths were 0.1 cm. Estimates of the magnitude of numerical diffusion were made by varying the zone widths and repeating the calculation. Changing the zone width by a factor of 2 produced a change of less than 5 % in computed results, leading to a conclusion that the numerical diffusion rate is substantially smaller than the physical diffusion rate in these problems. We can follow the progress of the flame front in Fig. 2, in which the temperature distribution and specific reaction rate are plotted as functions of position at two different times. The steep temperature rise in the flame region is spread over approximately four zones. The flame propagates because heat generated by the exothermic reaction is transported into the unburned region ahead of the flame, raising its temperature. The transport coefficients and the single reaction rate ($k = 1.1 \times 10^{13}\, e^{-30,000/RT}$ cm^3/mole-sec) were taken from Ref. [18]. Because of the relatively high activation energy in the reaction rate expression, the reactants will not burn until the temperature has reached a value of approximately 1500 K. The narrow reaction rate curves in Fig. 2 show that once the gas reaches that temperature the combustion is very rapid. Since the combustion chamber has a fixed volume and is assumed to be thermally insulated, the chamber pressure will rise as energy is released by reactions. During the time interval between the pairs of curves in Fig. 2, the average chamber pressure has increased from 35 to 50 atm. Even though the reaction rates in Fig. 2 are somewhat localized in space at each time, the sound speed in the gas is high enough that the pressure throughout the chamber is nearly uniform. These general features of the flame structure and propagation are reproduced by both models. In Fig. 3 we plot the

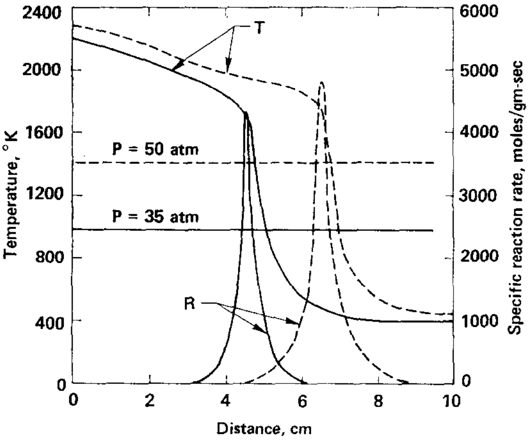

FIG. 2. Motion of flame front, showing temperature (T), pressure (P), and specific reaction rate (R). Solid lines indicate conditions at $t = 0.75$ msec, and dashed lines indicate conditions at 1.25 msec.

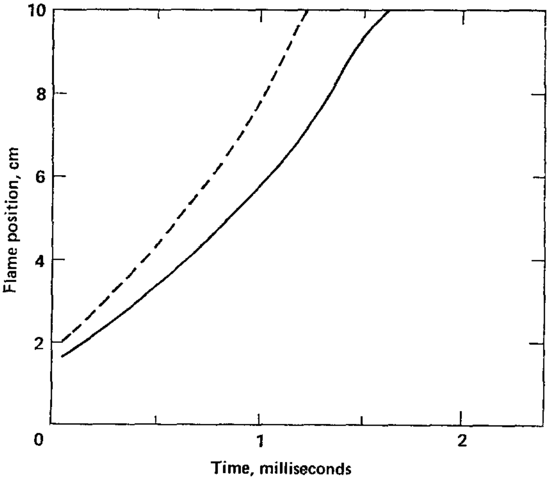

FIG. 3. Position of the flame front with time. Solid curve represents the generalized model results, and the dashed curve represents results using the conventional RICE operator splitting method.

position of the flame front as a function of time for both problems, with the ICE/RICE results indicated by the dotted curve, and the generalized model results indicated by the solid curve. The flame speeds are both typical of turbulent flames in closed, highly compressed combustion chambers. The curvature in the plots of flame position shows that the flame speed increases as the flame moves across the chamber. This acceleration is due to the fact that the flame compresses the unreacted gas ahead of the flame front and propagates into an increasingly dense medium. Since the reaction rate depends on the square of the density, the reaction rate steadily rises and accelerates the flame. It can be seen at once that the operator-split ICE/RICE model predicts a significantly higher propagation velocity for the flame than does the other model. An important result of this difference in flame speed is illustrated by Fig. 4 in which the total pressure is plotted for each model calculation as a function of time. Prediction of the pressure–time history of a combustion system is often the most important task of a numerical model, so the differences in behavior between the two models must be examined.

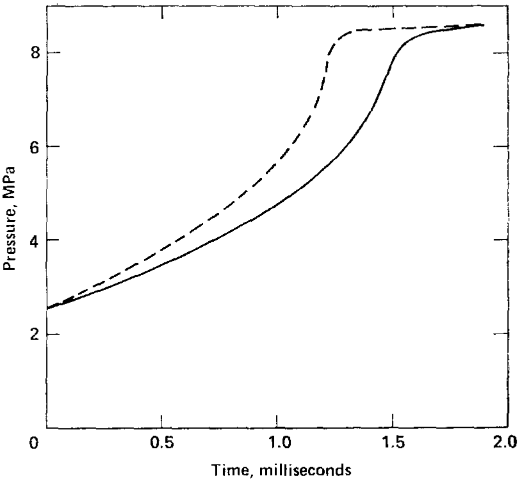

FIG. 4. Average combustion chamber pressure using the generalized model (solid curve) and the RICE splitting method (dashed curve).

From Eq. (10) we can write

$$\frac{\Delta P}{P} = \frac{\Delta\rho}{\rho} + \frac{\Delta T}{T} + \left(\sum_{l=1}^{L} \frac{\Delta Y_l}{A_l} \Big/ \sum_{l=1}^{L} \frac{Y_l}{A_l}\right), \tag{14}$$

where

$$\Delta P = P^{n+1} - P^n,$$

$$\Delta T = T^{n+1} - T^n,$$

$$\Delta\rho = \rho^{n+1} - \rho^n,$$

$$\Delta Y_l = Y_l^{n+1} - Y_l^{\,n}.$$

For a typical time step, we can plot each of the terms in Eq. (14) as functions of position in the combustion chamber. These curves, shown in Fig. 5, point out some important facets of deflagration waves. The last term in Eq. (14) is identically zero in these sample problems because of the single-step kinetics model. In calculations using a detailed chemical kinetics mechanism for methane oxidation [19], with 20 chemical species and 54 reactions, this term was also found to be negligible in comparison with the other terms in Eq. (14). Thus the primary effect which the chemical species kinetics and transport operators have upon the time advanced pressure is in releasing energy through chemical reactions and by transporting energy by diffusion, and not through changing the average molecular weight of the fluid and affecting the last term in Eq. (14). For the remaining terms, behind the flame in the product gases, and well ahead of the flame in the cold, unreacted region, we see that

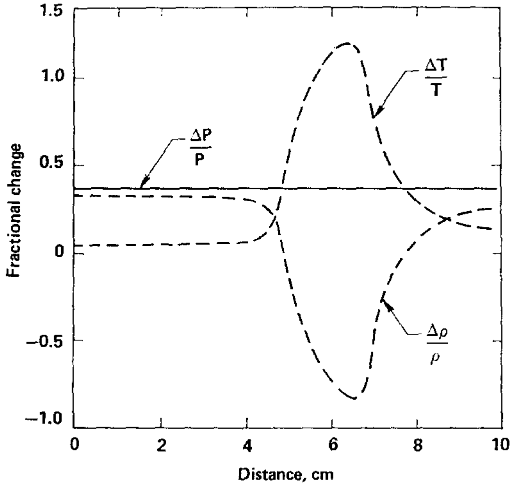

FIG. 5. Fractional changes in pressure ($\Delta P/P$), density ($\Delta\rho/\lambda$), and temperature ($\Delta T/T$).

$$\Delta\rho/\rho > \Delta T/T. \tag{15}$$

In such regions the majority of the pressure variation is a result of density variation. We would expect the ICE/RICE method to give a good estimate of $\bar{P}$ in those regions. Those regions are also characterized by the fact that the reaction rate and the energy deposition rate are both very small. However, in the reaction zone, where the energy release rate is large,

$$\Delta\rho/\rho < \Delta T/T. \tag{16}$$

In fact, Fig. 5 shows that there are regions where $\Delta\rho/\rho < 0$, although $\Delta P/P > 0$. One would expect the ICE/RICE method to have problems in these regions, since in these exothermic zones the ICE estimate of the pressure is a poor one.

It is interesting to see how the ICE method behaves in this flame region over a single time step. The zone pressures for several grid points ahead of and behind the flame are given in Table I. The first column gives P^n; the next column gives the pressure $\bar{P}$ used by the hydrodynamics subroutine; the third column gives the pressure following the chemical species transport; the next column gives the pressure after the chemical kinetics equations are advanced; the last column gives the final zone pressures P^{n+1}, following the solution of the energy equation. The temperature T^{n+1} is also included for comparison, to locate the flame region. Several important points may be made. First, the pressure is not truly uniform throughout the combustion chamber. Sound waves generated by the ignition process and by other physical and numerical properties of the flame propagation travel back and forth throughout the chamber. As a result the pressure at each grid point varies slightly about the average chamber pressure, which increases with time. Second, it is clear that $\bar{P}$ is not a good estimate of P^{n+1} in the flame region. The largest change in pressure is due to the exothermic reaction, which rapidly raises the temperature and pressure in the flame. Also note that in the flame region (zones 8–12) even the sign of the pressure change ($\bar{P} - P^n$) is not correct. Although the pressure in the flame region is increasing with time, the ICE hydrodynamics subroutine is misled into predicting a lower pressure in the flame. As a result of this erroneously lower pressure in the flame zone, an excessive mass flux from the hot burned gas region into the flame region and then into the unreacted gas region is computed. And even though subsequent operators for the chemical reactions and the energy equation approximately restore the pressure gradient, the

TABLE I

Summary of the Pressure Variations during a Single Time Step for a Flame Propagation Calculation Using the ICE/RICE Operator Splitting Scheme[a]

Zone	P^n	$\bar{P}_{\text{hydro}}$	$P_{\text{chemical transport}}$	$P_{\text{chemical kinetics}}$	P^{n+1}	T^{n+1}
5	35.767	36.327	36.327	36.661	36.475	2777
6	35.782	36.129	36.128	36.766	36.387	2639
7	35.939	35.948	35.947	37.195	36.430	2420
8	36.408	35.793	35.771	37.642	36.684	2065
9	36.155	35.577	35.593	36.386	36.872	1631
10	35.692	35.289	35.289	35.457	36.159	1312
11	35.096	34.919	34.920	34.956	35.569	1117
12	34.522	34.490	34.490	34.500	34.937	994
13	34.013	34.043	34.043	34.046	34.345	916
14	33.543	33.602	33.603	33.604	33.813	864
15	33.122	33.188	33.188	33.189	33.336	829

[a] Zones 5–7 have already burned, zones 8–12 are in the flame region, and zones 13–15 are not yet reacting.

erroneous mass flux is not corrected. The net result of this process is an overestimate of the energy transport due to convection into the flame region and into the unburned gas ahead of the flame. Thus the decoupling of the operators in the original ICE/RICE model introduces a biasing into the problem solution. By overestimating the net mass flux and heat flux ahead of the flame, the decoupled model predicts a propagation velocity for the flame which is too high.

Inclusion of the pressure changes due to heat release from chemical reactions in the new, generalized model serves two major purposes. Most important, the pressure used to compute the mass flux is always a good estimate of the actual time-advanced pressure. This eliminates systematic errors which have been seen to occur when the decoupled operator technique is used. Also, pressure oscillations during the course of a single time step, produced by the order in which the equations are solved in ICE/RICE, have been eliminated by the present coupled solution technique.

The rate of increase in the temperature in the flame region has been shown to play the key role in the systematic bias resulting from the ICE/RICE splitting scheme. In order to confirm this analysis, a second pair of calculations was made in which the reaction was 20% less exothermic than the first pair of calculations. The flame front positions for the RICE splitting scheme and the present model are shown in Fig. 6, and the overall results are compared in Table II. We see that the relative error between the RICE method and the present model decreases with decreasing reaction exothermicity. In the limit of very small exothermicity the two methods would give the same results. Furthermore, the dependence on relative exothermicity confirms the mechanism by which systematic biasing affects the calculations performed using the ICE/RICE splitting scheme.

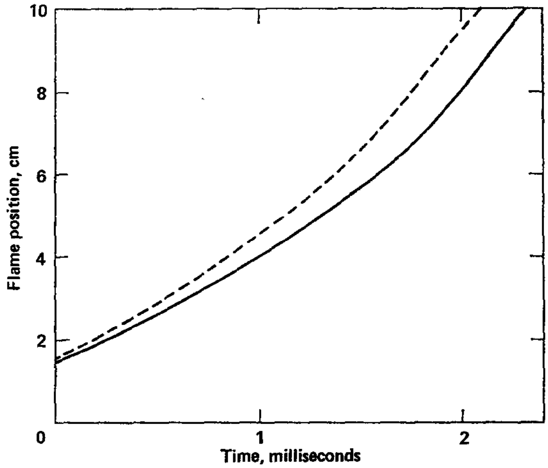

FIG. 6. Position of the flame front with time for the 20% less exothermic model. Solid curve represents the generalized model results, and the dashed curve represents the RICE splitting method results.

In both splitting schemes the time steps being used are nearly the same, about a factor of 10 larger than the Courant time step. Here the maximum time step is being controlled by accuracy considerations in the solution of the chemical kinetics equations. This type of time step limitation is very common in these combustion calculations. It is quite rare to find time step limitations resulting from the solution of the hydrodynamic equations, in either the ICE/RICE scheme or the present model. One might expect that the generalized model would exhibit enhanced stability characteristics and be able to run with larger time steps. But since chemical reaction time scales are almost invariably much shorter than the time steps allowed by either of the splitting schemes, this particular benefit of the generalized scheme is rarely realized. The major claim that is made for the generalized model is that the systematic biasing inherent in the ICE splitting scheme is avoided, at a very modest increase in computation time required. The generalized scheme requires 5–10% more computer time for the entire problem, with all of this time resulting from the higher number of times which the energy equation and chemical species equations must be solved, due to additional iterations. The average number of these iterations is usually less than five, and the maximum number of iterations commonly encountered during the course of an entire problem is between 15 and 20 iterations.

TABLE II

Comparison between RICE and the Present Generalized Model, Showing the Effects of Reaction Exothermicity[a]

Exothermicity (kcal/mole)	RICE	Present model	Relative error (%)
100	1.22	1.50	19
80	1.88	2.15	13

[a] The values in the columns labeled "RICE" and "Present model" are the times, in milliseconds, for the flame to propagate across the 10-cm combustion chamber.

CONCLUSION

The above generalization of the ICE method is intended to account for pressure dependence on other quantities in addition to density variations. The need for such a coupled treatment was originally motivated by observing the pressure variations at each grid point over a single time step which resulted from the ICE/RICE operator splitting scheme. It was subsequently discovered that systematic errors occurred in the ICE/RICE model for problems with significant energy deposition rates from exothermic chemical reactions. Both the pressure fluctuations over each time step and the systematic errors are eliminated in the new formulation. Larger time steps have not been observed with the new formulation because other operators are controlling the maximum allowable time step. Therefore, the new model uses the same time step as the conventional ICE/RICE model and requires very little additional computation time.

A general conclusion can be drawn from these results which may be useful in application areas beyond combustion problems. We have demonstrated that the ICE method should be used only in those situations in which the fluid pressure variations are due principally to density variations. In applications in which the pressure may change rapidly due to any other physical operator (e.g., exothermic chemical reactions, radiation energy deposition), it is not sufficient to split the pressure variation into a density-dependent part which is treated by ICE and another part which is treated subsequently. Such operators should be coupled inside the fluid dynamics formulation. If this is not done properly, systematic errors in the flow properties of the fluid will be produced as discussed above in the case of the planar deflagration wave. Finally, it should be reiterated that modification of most programs already using ICE/RICE and related techniques to the coupled form presented here should be quite simple in most cases.

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